Impurity Effects in Sign-Reversing Fully Gapped Superconductors: Analysis of FeAs Superconductors

Yuko Senga and Hiroshi Kontani
Department of Physics, Nagoya University, Furo-cho, Nagoya 464-8602, Japan.
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To understand the impurity effect on T_c in FeAs superconductors, we analyze a simple two-band BCS model with a repulsive interband interaction. The realized fully gapped superconducting state with sign reversal, which is predicted by spin fluctuation theories in this compound, is suppressed by impurities due to the interband hopping of Cooper pairs, if the interband impurity scattering I' is equal to the intraband one I. When $|I'/I| < 1$, in high contrast, T_c is almost unchanged by strong impurity scattering since interband scattering is almost prohibited by the multiple scattering effect. Since $|I'/I| \sim 0.5$ is expected, the robustness of superconductivity against impurities in FeAs superconductors is naturally understood in terms of the sign-reversing fully gapped state.

Keywords: iron pnictides, impurity effect, sign-reversing multiband superconductor

After the discovery of the superconductor La(O,F)FeAs (T_c = 26 K) [1], high-T_c superconductors with FeAs layers have been studied intensively [2–5]. The ground state of the undoped compound is the spin density wave (SDW) state, where the ordered magnetic moment is $\sim 0.3\ \mu_B$ and the ordering vector is $\mathbf{Q} \approx (\pi, 0)$ or $(0, \pi)$ [6–9]. The superconducting state is realized next to the SDW state by carrier doping [9, 10] According to NMR study, the singlet superconducting state is realized in FeAs [11–13]. In the first-principle band calculations [14, 15], the Fermi surfaces in FeAs are composed of two hole-like Fermi pockets around the $\Gamma = (0, 0)$ point (FS1 and FS2 in Fig. 3) and two electron-like Fermi pockets around M= $(\pi, 0), (0, \pi)$ points (FS3 and FS4 in Fig. 3).

Theoretically, there are several possible pairing states: According to the random phase approximation (RPA) based on a realistic five-orbital tight-binding model [16], the nesting between the hole and electron pockets gives rise to the strong antiferromagnetic (AF) fluctuations with $\mathbf{Q} \approx (\pi, 0)$, which is consistent with experimental results. Then, a fully gapped s-wave state with sign reversal is expected to emerge since AF fluctuations works as the repulsion interaction between hole and electron pockets [16–21]. Although AF fluctuations due to the nesting between two electron pockets [$\mathbf{q} \sim (\pi, \pi/2)$] can induce the $d_{x^2-y^2}$-wave state with line nodes on the hole pockets, the obtained T_c is rather low [16, 18–20]. On the other hand, the conventional s-wave state without sign reversal will be realized if the charge fluctuations or electron-phonon interactions are strong.

Experimentally, a fully gapped superconducting state has been determined by recent penetration depth measurement [22], angle-resolved photoemission spectroscopy (ARPES) [23–25], and specific heat measurement [26]. The resonance peak observed by inelastic neutron measurement below T_c supports the sign-reversing superconducting gap mediated by AF fluctuations [27, 28]. Anomalous transport phenomena (such as Hall coefficient and Nernst signal) in the normal state in FeAs, which are similar to those observed in high-T_c cuprates and CeMIn$_5$ (M=Co, Rh, Ir) [29], also indicate the existence of strong AF fluctuations [10, 12, 30, 31]. On the other hand, impurity effect on T_c due to Co, Ni, or Zn substitution for Fe sites is very small or absent [11, 12, 32–34], which is decisive for determining the pairing symmetry. For example, this result clearly rules out the possibility of line-node superconductivity. This result may also eliminate the theoretically predicted sign-reversing s-wave states, since the Cooper pair is destroyed by the interband scattering induced by impurities; $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)_{\rm band1} \to (\mathbf{k}'\uparrow, -\mathbf{k}'\downarrow)_{\rm band2}$. In this manner, a study of the impurity effect on FeAs superconductors offers us significant information on the pairing symmetry, and therefore reliable theoretical analyses are highly required.

In this letter, we study a simple two-band BCS model to investigate the impurity effect on FeAs superconductors. Therein, the sign-reversing pairing state is realized if we introduce the interband repulsive interaction to describe the effective interaction due to AF fluctuations. When the interband impurity scattering potential I' is equal to the intraband one I, the reduction in T_c per impurity concentration $n_{\rm imp}$, $-\Delta T_c/n_{\rm imp}$, is prominent as in non-s-wave superconductors. However, $x = |I'/I|$ is smaller than 1 in this compound since hole and electron pockets are not composed of the same d-orbitals. In this case, $-\Delta T_c/n_{\rm imp}$ becomes very small; in particular, it approaches *zero* in the unitary regime ($I/W_{\rm band} \gg 1$). Therefore, the experimental absence of the impurity effect on T_c in FeAs is well understood in terms of the sign-reversing s-wave state proposed in refs. [16] and [17].

Here, we analyze the Eliashberg gap equation for the two-band BCS model. To concentrate on studying the impurity effect, we neglect the mass-enhancement factor and the quasiparticle damping due to electron-electron interaction for simplicity, both of which are given by the

normal self-energy. In the absence of impurities, the linearized gap equation at T_c is given by [35]:

$$\Delta_i(p_n) = -\pi T_c \sum_{j=\alpha,\beta} g_{ij} N_j \sum_m{}' \Delta_j(p_m)/|p_m|, \quad (1)$$

where p_n, p_m are fermion Matsubara frequencies, and i, j $(= \alpha, \beta)$ are band indices. N_i is the density of states at the Fermi level, and g_{ij} is the effective interaction between band i and band j. $\sum'_m \equiv \sum_m \theta(\omega_c - |p_m|)$, where ω_c is the characteristic energy scale of the effective interaction. $\Delta_i(p_n)$ is the gap function, which is independent of p_n for $|p_n| < \omega_c$ in the absence of impurities. Hereafter, we assume $g_{\alpha\beta} \equiv g > 0$ to realize the sign-reversing s-wave gap ($\Delta_\alpha \Delta_\beta < 0$), and put $g_{\alpha\alpha} = g_{\beta\beta} = 0$ for simplicity since they will be much smaller than g in FeAs. After the standard analysis [35], the transition temperature without impurities is obtained as $T_c^0 = 1.13\omega_c \exp(-1/g\sqrt{N_\alpha N_\beta})$.

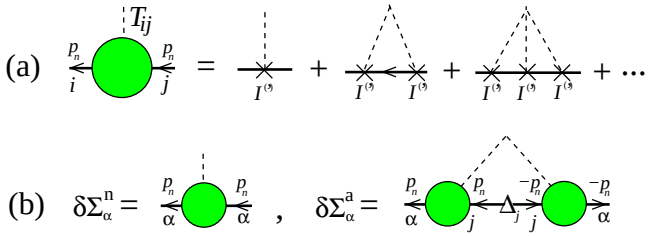

FIG. 1: (a) T-matrix in the normal state. (b) Impurity-induced normal self-energy ($\delta\Sigma_\alpha^n$) and the linealized anomalous self-energy ($\delta\Sigma_\alpha^a$) in the T-matrix approximation.

Hereafter, we study the nonmagnetic impurity effect in the two-band BCS model with $g_{\alpha\beta} > 0$. In similar models, the effect of interband impurity scattering in the NMR relaxation ratio has been analyzed using the Born approximation [36] and T-matrix approximation for $I = I' = \infty$ [37]. Very recently, Bang et al. have reported a sizable reduction in T_c by a strong impurity potential with $I = I'$ [38]. In contrast to their result, we will show below that T_c is almost unchanged when $I'/I < 1$.

Hereafter, we use the T-matrix approximation, which gives the exact result for $n_{\rm imp} \ll 1$ for any strength of I, I'. We can assume that $I, I' \geq 0$ without losing generality. Using the local normal Green function $g_i(p_n) = -i\pi N_i s_n$ ($s_n \equiv {\rm sgn}(p_n)$) [35], the T-matrix in the normal state is given by

$$T_{ij}(p_n) = I_{ij} + \sum_{l=\alpha,\beta} I_{il} g_l(p_n) T_{lj}(p_n), \quad (2)$$

where $I_{ij} = I\delta_{i,j} + I'(1-\delta_{i,j})$. Its diagrammatic expression is shown in Fig. 1 (a). Except at $x = 1$, the solution of eq. (2) behaves as $T_{\alpha\alpha} \sim -is_n/\pi N_\alpha + O(I^{-1})$ and $T_{\alpha\beta} \sim O(I^{-1})$ in the unitary limit. This fact means that the *the superconducting state is unaffected by a strong impurity potential since the interband scattering is prohibited as a result of multiple scattering.*

Using the T-matrix, the impurity-induced normal and anomalous self-energies are respectively given as

$$\delta\Sigma_i^n(p_n) = n_{\rm imp} T_{ii}(p_n), \quad (3)$$

$$\delta\Sigma_i^a(p_n) = n_{\rm imp} \sum_{l=\alpha,\beta} T_{il}(p_n) f_l(p_n) T_{li}(-p_n), \quad (4)$$

where $f_i(p_n) \equiv \pi N_i \Delta_i(p_n)/|p_n|$ is the local anomalous Green function at T_c. Their expressions are shown in Fig. 1 (b). Then, the gap equation at T_c is given by [35]

$$Z_i(p_n)\Delta_i(p_n) = -\pi T_c \sum_{j=\alpha,\beta} g_{ij} N_j \sum_m{}' \Delta_j(p_m)/|p_m| + \delta\Sigma_i^a(p_n), \quad (5)$$

where $Z_i(p_n) \equiv 1 - (\delta\Sigma_i^n(p_n) - \delta\Sigma_i^n(-p_n))/2ip_n = 1 + \gamma_i/|p_n|$, and $\gamma_i = -{\rm Im}\Sigma_i^n(p_n) \cdot s_n$ (> 0) is the quasiparticle damping rate due to impurity scattering.

Now, we analyze the impurity effect on T_c in the case of $N_\alpha = N_\beta \equiv N$ as the first step. In this case, the relationships $\gamma_\alpha = \gamma_\beta \equiv \gamma$, $\Delta_\alpha(p_n) = -\Delta_\beta(p_n) \equiv \Delta(p_n)$, and $\delta\Sigma_\alpha^a = -\delta\Sigma_\beta^a \equiv \delta\Sigma^a$ are satisfied. They are obtained as

$$\gamma = n_{\rm imp}\pi N[(I^2 + I'^2) + \pi^2 N^2 (I^2 - I'^2)^2]/A, \quad (6)$$

$$\delta\Sigma^a(p_n) = n_{\rm imp}\Delta(p_n)\pi N[(I^2 - I'^2) + \pi^2 N^2 (I^2 - I'^2)^2]/|p_n|A, \quad (7)$$

where A is defined as

$$A = 1 + 2\pi^2 N^2 (I^2 + I'^2) + \pi^4 N^4 (I^2 - I'^2)^2. \quad (8)$$

We will show below that the interband impurity scattering I' is renormalized by $1/\sqrt{A}$. Using eqs. (5)-(8), the frequency dependence of the gap function is obtained as

$$\Delta(p_n) = C\left[Z(p_n) - \delta\Sigma^a(p_n)/\Delta(p_n)\right]^{-1} = C\left[1 + 2n_{\rm imp}\pi N I'^2/|p_n|A\right]^{-1}, \quad (9)$$

where $C \equiv \pi N g T_c \sum'_m \Delta(p_m)/|p_m|$ is a constant independent of p_n. By inserting eq. (9) into the definition of C, we obtain the following equation for T_c:

$$1 = \pi N g T_c \sum_m{}' \left[|p_m| + 2\pi n_{\rm imp} N I'^2/A\right]^{-1} = gN\left[\ln\frac{\omega_c}{2\pi T_c} - \psi\left(\frac{1}{2} + \frac{n_{\rm imp} N I'^2}{T_c A}\right)\right], \quad (10)$$

where $\psi(x)$ is the digamma function. The equation for T_c^0 is given by dropping the term $n_{\rm imp} N I'^2/T_c A$ in eq. (10). It is noteworthy that this term also vanishes when $x \neq 1$ and $I \to \infty$, even if $n_{\rm imp} > 0$. This fact means

that superconducting state is unaffected by impurities in the unitary limit.

Using eq. (10) and the relation $\psi'(1/2) = \pi^2/2$, we obtain the relationship $\ln(T_c^0/T_c) = n_{\rm imp}\pi^2 N I'^2/2T_c^0 A$ for $n_{\rm imp} \ll 1$. As a result, the reduction in T_c per impurity concentration for $n_{\rm imp} \ll 1$ is obtained as

$$-\frac{\Delta T_c}{n_{\rm imp}} = \frac{\pi^2 N I'^2}{2A}. \tag{11}$$

The physical meaning of the right-hand side of eq. (11) is the rate of pair breaking, which is given by the amplitude of interband scattering for Cooper pairs: $|T_{\alpha\beta}|^2$. Its I dependence is shown in Fig. 2 (a). When $x = 1$, eq. (11) increases in proportion to I^2 in the Born regime ($\pi IN \ll 1$), and it approaches $1/8N$ in the unitary regime ($\pi IN \gg 1$). In the latter case, the superconductivity in FeAs will be destroyed only at $n_{\rm imp} \approx 8NT_c^0 \sim 0.02$ since the average between the electron and hole density of states per Fe atom is 0.66 eV^{-1} [14]. When $x \neq 1$, in contrast, eq. (11) $\approx x^2/2\pi^2 N^3 I^2(1-x^2)^2 \to 0$ in the unitary limit. In this case, pair breaking is almost absent and T_c is unchanged.

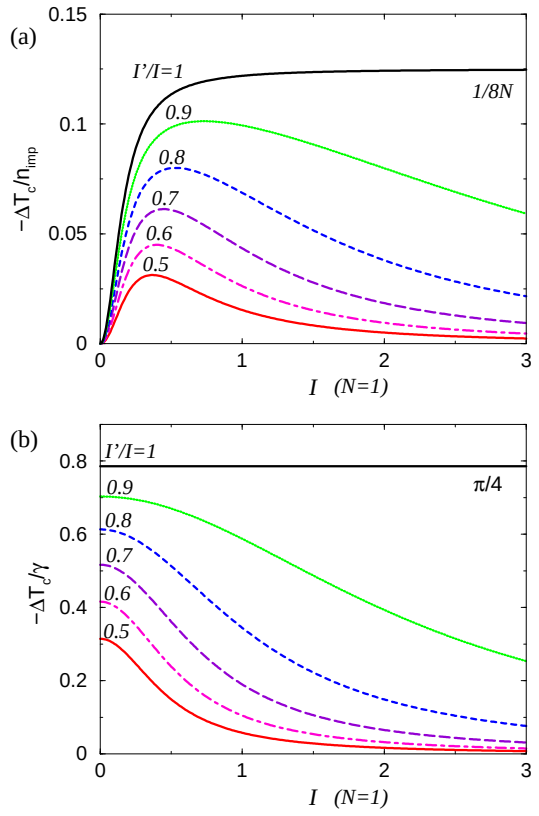

FIG. 2: (a) $-\Delta T_c/n_{\rm imp}$ and (b) $-\Delta T_c/\gamma$ as functions of I. $1/8N \sim 2500$ K in FeAs. When $x < 0.8$, $-\Delta T_c$ becomes very small for $I \gtrsim 3$.

According to eqs. (11) and (6), we obtain as

$$-\frac{\Delta T_c}{\gamma} = \frac{\pi x^2}{2(1+x^2) + 2\pi^2 N^2 I^2 (1-x^2)^2}. \tag{12}$$

In the Born limit, $-\Delta T_c/\gamma = \pi x^2/2(1+x^2)$, which diminishes slowly as x decreases from unity. In the unitary limit, it is strongly suppressed as $-\Delta T_c/\gamma \sim [-\Delta T_c/\gamma]_{\rm Born} \times (\pi NI)^{-1} \to 0$ for $x \neq 1$. Note that γ is related to residual resistivity as $\rho_0 = 2m\gamma/e^2 n$, where n is the carrier density. Figure 2 (b) shows the I dependence of eq. (12): For $x = 0.5$, $-\Delta T_c/\gamma = 0.0077$ at $IN = 3$, which is two orders of magnitude smaller than $\pi/4$. Such a small impurity effect will be difficult to observe experimentally.

Next, we discuss the case of $N_\alpha \neq N_\beta$, where the relation $\Delta_\alpha = -\Delta_\beta$ is not satisfied. Even in this case, we can obtain $-\Delta T_c/n_{\rm imp}$ by solving eq. (5) analytically. After a long calculation, the obtained result for $n_{\rm imp} \ll 1$ is

$$-\frac{\Delta T_c}{n_{\rm imp}} = \frac{\pi^2 \left[\, 3(N_\alpha + N_\beta) - 2\sqrt{N_\alpha N_\beta}\,\right] I'^2}{8\bar{A}}, \tag{13}$$

where $\bar{A} = 1 + \pi^2 I^2 (N_\alpha^2 + N_\beta^2) + 2N_\alpha N_\beta \pi^2 I'^2 + N_\alpha^2 N_\beta^2 \pi^4 (I^2 - I'^2)^2$, which is proportional to $I^4(1-x^2)^2$ in the unitary regime. Therefore, eq. (13) approaches zero in the case of $x \neq 1$ in the unitary regime. Thus, the obtained results for $N_\alpha = N_\beta$ given in Fig. 2 are qualitatively unchanged even for $N_\alpha \neq N_\beta$.

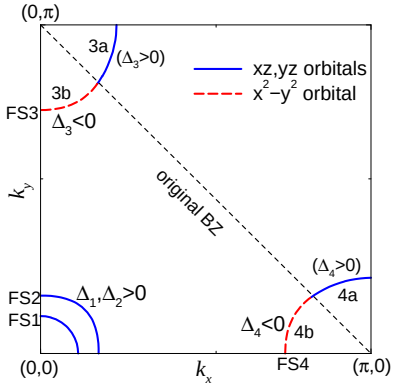

FIG. 3: Fermi surfaces (FSs) in FeAs superconductors in the unfolded Brillouin zone; see ref. [16].

On the basis of the above results, we discuss the impurity effect on T_c in real FeAs superconductors. Figure 3 shows the Fermi surfaces (FS1-FS4) of this compound in the unfolded Brillouin zone [16, 17]: FS1,2 are mainly composed of d_{xz}, d_{yz} orbitals of Fe, whereas FS3,4 are composed of d_{xz}, d_{yz} and $d_{x^2-y^2}$ orbitals, according to the five-orbital model in ref. [16]. More precisely, FS3a,4a (3b,4b) are composed of d_{xz}, d_{yz} orbitals ($d_{x^2-y^2}$ orbital). Mazin et al. had proposed that superconducting gap functions in FS1,2 ($\Delta_{1,2}$) and those in FS3,4 ($\Delta_{3,4}$) are

different in sign. In this case, bands α and β in the present study correspond to FS1,2 and FS3,4 in FeAs, respectively.

Here, we consider an impurity d-atom (such as Co, Ni, or Zn) placed at an Fe site. In the d orbital representation, the local impurity potential will be diagonal with respect to the d orbital $d(d')$: $(\hat{I})_{d,d'} = I\delta_{d,d'}$. In the band-diagonal representation, it is transformed into

$$I_{ij} \approx I\langle\sum_{d} O_{d,i}(\mathbf{k})O_{d,j}(\mathbf{k}')\rangle^{\rm FS}_{\mathbf{k}\in\alpha,\mathbf{k}'\in\beta}, \qquad (14)$$

where i,j $(=\alpha,\beta)$ represent the band indices. $O_{d,i}(\mathbf{k}) \equiv \langle d;\mathbf{k}|i;\mathbf{k}\rangle$ is the transformation orthogonal (or unitary) matrix between the orbital representation (orbital d) and the band-diagonal representation (band i). Therefore, $I_{\alpha\alpha}$, $I_{\beta\beta} \approx I$ whereas $|I_{\alpha\beta}|$ should be smaller than $|I|$ when bands α and β are composed of different d orbitals. Since FS3b,4b are composed of $d_{x^2-y^2}$ orbitals of Fe, the relation $x = |I'/I| \sim 0.5$ is realized in FeAs.

On the other hand, according to the RPA analysis by Kuroki et al. [16], $\Delta_{3,4}$ has line nodes near $(\pi,0)-(0,\pi)$ line owing to spin fluctuations with $\mathbf{q} \approx (\pi,\pi/2)$; therein, the sign of $\Delta_{3,4}$ for FS3a,4a (3b,4b) and that of $\Delta_{1,2}$ are equal (different). Then, bands α and β in the present study correspond to [FS1,2+3a,4a] and [FS3b,4b] in FeAs, respectively. Since bands α and β are composed of different d orbitals, the relation $x \ll 1$ is expected. Note that the obtained s-wave state is fully gapped since the line nodes on FS3,4, which are not protected by symmetry, are masked by small interband pairing [16]. We also note that the sign change in $\Delta_{3,4}$ does not occur and Mazin's type sign-reversing state is realized in the case of $U \approx U'$ [16].

As a result, in both unconventional s-wave states proposed in refs. [16] and [17], $-\Delta T_{\rm c}/\gamma^{\rm imp} \approx 0$ in the unitary regime. In high-$T_{\rm c}$ cuprates, I due to Zn impurity is about 10 eV [31]. If we expect $I \sim 10$ eV and $N_{\alpha,\beta} \sim 1$ eV^{-1} in FeAs, the unitary regime is actually achieved.

Although we have put $g_{\alpha\alpha} = g_{\beta\beta} = 0$ above, they will take positive (negative) values owing to electron-electron correlation (electron-phonon interaction) in FeAs superconductors. Although these diagonal interactions modify $T_{\rm c}^0$, we can show that both eqs. (11) and (12) are unchanged even if $g_{\alpha\alpha}, g_{\beta\beta} \neq 0$. Thus, the obtained results in the present study will be valid for general multiband fully gapped superconductors with sign reversal.

In summary, we analyzed the impurity effect on $T_{\rm c}$ in a sign-reversing s-wave BCS model. Except at $I' = I$, $T_{\rm c}$ is almost unaffected by impurities in the unitary limit, since the interband elements of the T-matrix vanish due to multiple scattering. Thus, the robustness of superconductivity against Co, Ni, or Zn impurities in this compound is naturally explained in terms of the sign-reversing s-wave superconductivity [16–21]. On the other hand, a weak impurity scattering causes pair breaking. Therefore, the finite density of states may be induced in the superconducting state by weak impurities or disorder.

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